Glassiness Vs. Order in Densely Frustrated Josephson Arrays

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We carry out extensive Monte Carlo simulations of the Coulomb gas dual to the uniformly frustrated two dimensional XY model, for a sequence of frustrations f converging to the irrational $(3-\sqrt{5})/2$. We find in these systems a sharp first order equilibrium phase transition to an ordered vortex structure at a T_c which varies only slightly with f. This ordered vortex structure remains in general phase incoherent until a lower vortex pinning transition $T_p(f)$ that varies with f. We argue that the glassy behaviors reported for this model in earlier simulations are dynamic effects.

64.70.Pf, 64.60.Cn

The glass transition to a frozen disordered state remains one of the oldest unresolved problems of condensed matter physics. While much progress had been made in the area of "spin glasses", in which the glassy state is a consequence of intrinsic random frustration in the Hamiltonian, the problem of "structural glasses", which possess no intrinsic random disorder, remains poorly understood [1,2]. It is therefore desirable to search for glasslike transitions in simple intrinsically disorder-free statistical models. One such candidate system is the two dimensional (2D) *uniformly frustrated* XY model, which models a periodic array of Josephson junctions in a transverse applied magnetic field [3,4]. Varying the frustration parameter f (magnetic field) of this model leads to complex commensurability effects between the underlying discrete grid and the vortex lattice that forms in response to the frustration [5]. Some years ago, Halsey [6] presented numerical evidence that, in the limit of an irrational $f^* = (3-\sqrt{5})/2$, this model displays a finite temperature glass transition T_g to a superconducting frozen disordered vortex state [7]. Experiments on superconducting wire networks with Halsey's irrational f^* have found evidence for a finite T_g from the scaling of current-voltage (IV) characteristics [8]. However simulations by Granato [9], using resistively shunted junction dynamics, found an IV scaling consistent with $T_g = 0$. Recently, Kim and Lee [10] have re-investigated this problem using Langevin simulations. They find that near Halsey's T_g, the system's dynamics resembles the primary relaxation of supercooled liquids rather than that of a spin glass.

In view of the above conflicting results, it is important to establish the true equilibrium behavior of this model. We therefore re-investigate Halsey's problem by carrying out Monte Carlo (MC) simulations of the 2D Coulomb gas which is dual to the uniformly frustrated XY models. Working with vortex variables directly allows us greater control over the most relevant slow variables involved in equilibration, as compared to using the phase variables of the original XY model [6,7,9,10]. Following Halsey, we consider the frustrations $f = 5/13$, $8/21$, $13/34$, and $21/55$, which are the first few members of a Fibonacci sequence of rational approximants which converges to the irrational $f^* = (3-\sqrt{5})/2$. We find that the low temperature state that is reached upon slow cooling is highly sensitive to both the dynamics used as well as the system length L. The true ground states for such $f = p/q$ are much more complex than previously believed, even for relatively small values of q. We find that when next-nearest-neighbor vortex hops are included in the dynamics, all cases show clear evidence for a sharp *first order* equilibrium phase transition T_c near Halsey's T_g, to an *ordered* vortex structure consisting of completely filled, completely empty, and partially filled diagonals. Below T_c, vortices in the partially filled diagonals can remain mobile, destroying phase coherence in the direction transverse to the diagonal. These vortices pin to the grid, leading to phase coherence in all directions, only at a lower $T_p(f)$ that varies with f. We therefore conclude that the "glass transition" observed by Halsey, and the supercooling observed by Kim and Lee, is a consequence of energy barriers in their particular dynamics inhibiting what is a true first order equilibrium phase transition to a non-glassy ordered state.

The uniformly frustrated 2D XY model, within the Villain approximation [11], can be mapped [12] onto the following Hamiltonian for a one component Coulomb gas on a neutralizing background,

$$\mathcal{H}_{\rm CG}[n_i] = \frac{1}{2}\sum_{i,j}(n_i - f)G'(\mathbf{r}_i - \mathbf{r}_j)(n_j - f) \ . \qquad (1)$$

The sum is over all sites of a 2D periodic square $L \times L$ grid. n_i is the integer charge on site i, representing the vorticity of the XY phase angle. The frustration parameter f, acting as a background charge density, represents the density of flux quanta in the applied magnetic field. The interaction is $G'(\mathbf{r}) = G(\mathbf{r}) - G(\mathbf{0})$, where $G(\mathbf{r})$ is the lattice Coulomb potential in 2D, with periodic boundary conditions. Charge neutrality, $\sum_i n_i = L^2 f$, is imposed. See Ref. [13] for further details.

The elementary move of our MC procedure is the insertion of a randomly positioned vortex-antivortex pair, $\Delta n_i = +1$, $\Delta n_j = -1$, which is then either accepted or

rejected by a standard Metropolis algorithm. When we restrict i and j to nearest-neighbor sites, we find glassy results qualitatively similar to Halsey's. When we allow i and j to include next-nearest-neighbor sites as well, we find equilibration at low temperatures to be dramatically improved. Our results below are for this latter dynamics. Simulations were carried out cooling from an initial random configuration. At each temperature 20,000 initial MC passes are discarded for equilibration, with an additional 1,280,000 MC passes for computing averages. One MC pass refers to L^2 elementary moves.

In Fig. 1 we show intensity plots for the *average* vorticity at each site, at $T = 0.02 < T_c \simeq 0.03$. Black squares are sites with $\langle n_i \rangle \simeq 0$; white squares are sites with $\langle n_i \rangle \simeq 1$; gray squares are sites with an average vortex occupation of $0 < \langle n_i \rangle < 1$. We find an ordered sequence of completely filled, completely empty, and partially filled diagonals, clearly different from the disordered structures found by Halsey. For Figs. 1a,c,d, we find translational invariance along the diagonals, except for occasional defects. For $f = 8/21$ (Fig. 1b) the partially filled diagonals have a pinned vacancy on every third site.

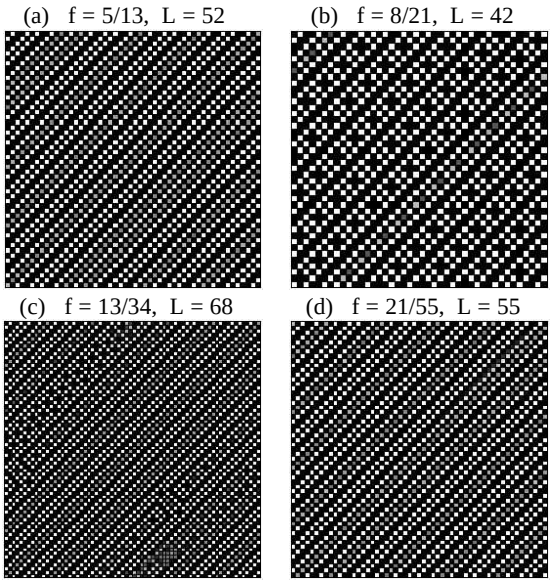

FIG. 1. Intensity plot of ordered vortex states at $T = 0.02 < T_c$. White squares contain vortices, black squares contain no vortices, and gray squares have an average vortex occupation of $0 < \langle n_i \rangle < 1$.

We do not know that the states shown in Fig. 1 represent the true ordered states in the thermodynamic limit. For $f = 5/13$, for example, using $L = 26$ and $L = 52$ resulted in a differing sequence for the filled, empty, and partially filled diagonals. For $f = 8/21$, the vortices in the partially filled diagonals occupy exactly 2/3 of the sites in these diagonals. We may speculate that in the true ground state these vortices will from a periodic lattice with the same structure as the $f = 2/3$ ground state [3]. Such a structure can only be made perfectly periodic, and commensurate with the periodicity of the diagonals, when L is an integer multiple of 84. The structure shown in Fig. 1b, with $L = 42$, consists of such an $f = 2/3$–like arrangement, however with a domain wall introduced by our choice of a too small value of L. From such considerations we conclude that the true ground state, for all but the simplest of $f = p/q$, may involve rather subtle and *a priori* unknown commensurability requirements; its square unit cell will be of length mq where m may well be an integer several times larger than previously believed [14].

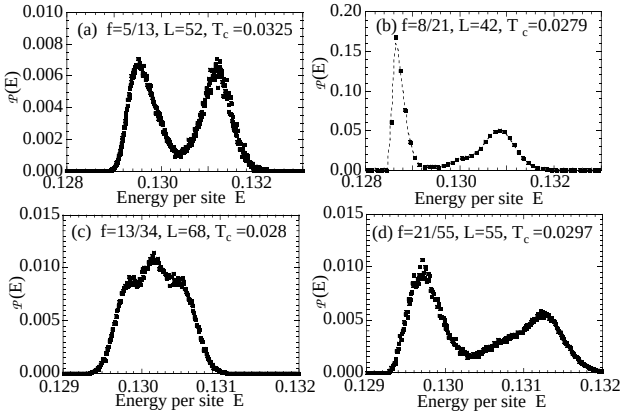

FIG. 2. Bimodal energy distribution $\mathcal{P}(E)$ at T_c. The first order transition temperature $T_c \simeq 0.03$ is fixed by the condition that the peaks subtend equal areas.

For each case we find that the transition to the ordered state is sharp and seemingly first order. To demonstrate this, we compute the histogram of energies $\mathcal{P}(E)$ encountered at each value of temperature in the simulation. In both high and low temperature regions, this histogram is unimodal. However in a narrow temperature range when the ordered state first appears, the distribution becomes bimodal corresponding to the two coexisting states at a first order transition. Using an extrapolation technique [15] we determine T_c as the temperature for which the two peaks of the bimodal histogram subtend equal *area* [16]. Our results are shown in Fig. 2. For Figs. 2a,b,d, the two peaks are well separated; the less clear case of $f = 13/34$ is perhaps a reflection of the larger concentration of defects seen in Fig. 1c, or the possibility that our size $L = 68$ still gives too poor an approximation of the true ground state. In the mapping from the XY model to the Coulomb gas the temperature has been rescaled [13] so that $T^{\rm XY} = 2\pi T^{\rm CG}$. Our value $T_c^{\rm CG} \simeq 0.03$ is thus reasonably close to Halsey's value of $T_g^{\rm XY} \simeq 0.25$.

Next we consider the superconducting phase coherence of the Josephson array. In the original uniformly frustrated XY model of phase angles θ_i, the issue of phase coherence may be addressed by considering the dependence of the total free energy $\mathcal{F}$ on the net phase angle twist Δ_μ that is applied across the sample as a boundary

condition, i.e. $\theta(\mathbf{r}_i + L\hat{\mu}) = \theta(\mathbf{r}_i) + \Delta_\mu$. If $\mathcal{F}[\Delta_x, \Delta_y]$ is independent of the Δ_μ, then phase coherence is lost. Doing the duality transformation to the Coulomb gas carefully [12,17,18], one finds that such a fixed twist boundary condition results in an additional term to the Coulomb gas Hamiltonian of Eq. (1),

$$\delta\mathcal{H}[\mathbf{p}; \Delta_x, \Delta_y] = V(\frac{2\pi p_x}{L} - \Delta_y) + V(\frac{2\pi p_y}{L} + \Delta_x) \quad (2)$$

where

$$\mathbf{p} = \sum_i \mathbf{r}_i n_i \quad (3)$$

is the total "dipole moment" of the vortices, and

$$V(\phi) = -T \ln \left[\sum_{m=-\infty}^{\infty} e^{-\frac{1}{4\pi T}(\phi - 2\pi m)^2} \right] \quad (4)$$

is the Villain function [11] with coupling $2\pi T$. The partition function for the system with a fixed twist Δ_μ is then $Z[\Delta_x, \Delta_y] = Z_{\rm CG} \langle e^{-\delta\mathcal{H}[\mathbf{p};\Delta_x,\Delta_y]/T} \rangle$. Here $Z_{\rm CG}$ is the partition function for the ensemble defined by $\mathcal{H}_{\rm CG}$ of Eq. (1) alone, and the average is with respect to this ensemble ($\mathcal{H}_{\rm CG}$ can be considered as the ensemble in which Δ_μ is averaged over, and so one has "fluctuating twist boundary conditions" in the XY model [17]). The total free energy is then $\mathcal{F}[\Delta_x, \Delta_y] = \mathcal{F}_{\rm CG} + \delta\mathcal{F}[\Delta_x, \Delta_y]$, where $\mathcal{F}_{\rm CG} = -T \ln Z_{\rm CG}$ and

$$\delta\mathcal{F}[\Delta_x, \Delta_y] = -T \ln \sum_{p_x, p_y} \mathcal{P}(p_x, p_y) e^{-\delta\mathcal{H}[\mathbf{p};\Delta_x,\Delta_y]/T} \quad (5)$$

where $\mathcal{P}(p_x, p_y)$ is the histogram of total dipole moments $\mathbf{p}$ at a given temperature, found in the simulation using $\mathcal{H}_{\rm CG}$ of Eq. (1). By storing this 2D histogram, we can therefore deduce the dependence of the free energy on *all* values of applied twist Δ_μ.

In Fig. 3 we show intensity plots of $\delta\mathcal{F}[\Delta_x, \Delta_y]$ for $\Delta_\mu \in (-\pi, \pi)$ at $T = 0.02 < T_c$, corresponding to the real space plots of Fig. 1. For $f = 8/21$, Fig. 3b, we see a rotationally symmetric parabolic minimum indicating that the system is phase coherent in all directions (that there are actually two such minima, is a result of the thermal motion of the domain wall inserted by our choice of $L = 42$). For the other cases however, we see that while $\delta\mathcal{F}$ has a parabolic minimum along the direction parallel to the ordered diagonals, it is constant for the direction perpendicular to these diagonals. This indicates that the vortices in the partially filled diagonals are free to move along these diagonals and so destroy phase coherence transverse to this direction. Noting that an applied electric current exerts a force on the vortices which is transverse to the direction of the current, we would expect the Josephson array to have a finite linear resistivity for all cases except when the current is applied exactly parallel to the partially filled diagonals. Thus the structural transition at T_c is not in general the superconducting transition of the array.

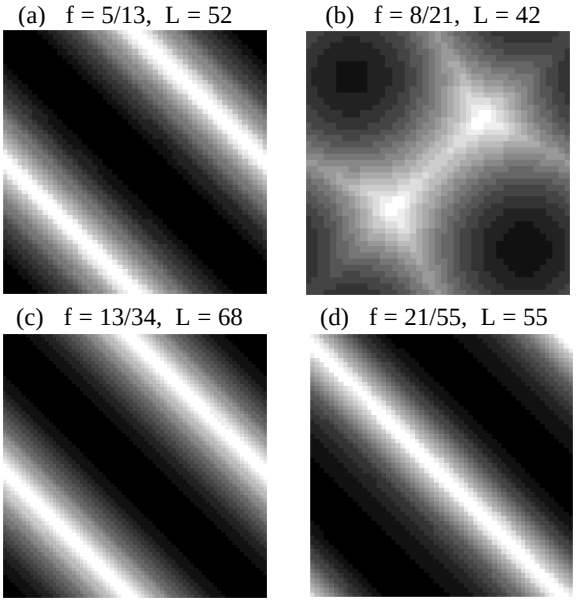

FIG. 3. Intensity plot of total free energy $\delta\mathcal{F}[\Delta_x, \Delta_y]$ at $T = 0.02 < T_c$. Black (white) denotes the functional minima (maxima).

The helicity modulus tensor $\Upsilon_{\mu\nu}$ of the 2D XY model is defined by [19]

$$\Upsilon_{\mu\nu} \equiv \frac{\partial^2 \mathcal{F}}{\partial\Delta_\mu \partial\Delta_\nu} \quad (6)$$

where the derivatives are evaluated at the value $\Delta_{\mu 0}$ that minimizes $\mathcal{F}$. From Fig. 3 we expect that $\Upsilon_{\mu\nu}$ is diagonal in a basis that is aligned with the grid diagonal directions. We therefore denote by $\Upsilon_\perp$ and $\Upsilon_\parallel$ the eigenvalues of $\Upsilon_{\mu\nu}$ in the directions perpendicular and parallel to the ordered diagonals respectively. In Fig. 4 we plot $\Upsilon_\perp$ and $\Upsilon_\parallel$ as functions of T, for the same values of f and L as in Figs. 1 and 3. As expected from Fig. 3 we see that for all cases $\Upsilon_\parallel$ increases from zero as T decreases below T_c. However, except for the case $f = 8/21$, $\Upsilon_\perp$ remains zero below T_c, becoming non-zero only at a lower temperature $T_p(f)$ when the vortices in the partially filled diagonals pin to the grid. Similar behavior, of mobile vortex "defects" in an otherwise ordered vortex structure, has been observed previously [20] in simulations of the $f = 5/11$ model. If the vortices in the partially filled diagonals remain mutually correlated, the region $T_p(f) < T < T_c$ can be described as a "floating smectic" phase, as first postulated by Ostlund [21]. If however the correlations are short ranged, as in a liquid, one might imagine that vortex hopping between the different partially filled diagonals may also be possible. In this case, our result that $\Upsilon_\parallel > 0$ for $T_p(f) < T < T_c$ might be a reflection of the very high energy barrier for such inter-diagonal hops, rather than a true phase coherence effect.

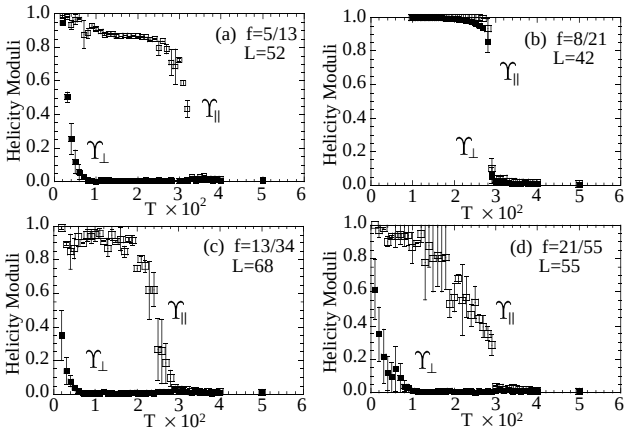

FIG. 4. Helicity modulus eigenvalues $\Upsilon_\parallel$ and $\Upsilon_\perp$ vs. T. $\Upsilon_\parallel$ is non-zero below $T_c \simeq 0.03$, however $\Upsilon_\perp$ is non-zero only below $T_p(f) \leq T_c$.

We conclude that the sequence of rational f that approach the irrational $f^* = (3-\sqrt{5})/2$ all undergo a first order equilibrium phase transition to an ordered vortex structure at a $T_c \simeq 0.03$. The exact sequence of the filled, empty, and partially filled diagonals in this ordered structure remains in general unknown for the true ground state in the thermodynamic limit, however in the cases when we varied $L = mq$ for fixed $f = p/q$, we found that T_c remained approximately 0.03. The transition to the true superconducting state, with phase coherence in all directions, occurs in general at a lower $T_p(f)$, which can show considerable variation with the frustration f. While this is in qualitative agreement with arguments by Teitel and Jayaprakash [3], which suggested that the superconducting transition temperature would be a very discontinuous function of f, we as yet can discern no systematic dependence on $f = p/q$ nor can we be certain that the values of $T_p(f)$ obtained here will not vary if one increases the system size L.

Our equilibrium transition at T_c to an ordered vortex structure was only obtained when we included next-nearest-neighbor hops in our vortex dynamics. When moves were restricted to nearest-neighbor hops only, our simulations fell out of equilibrium into a frozen disordered state below $T \simeq 0.033$. Fig. 1 suggests why this is so. Next-nearest-neighbor hops allow vortices to travel directly up and down the partially filled diagonals. To make such a move using only nearest-neighbor hops, one must first hop to a neighboring diagonal, putting three vortices mutually adjacent. We find for the energy barrier of such moves $\Delta E \simeq 0.23 - 0.35$, depending on f, and so these moves tend to freeze out by the temperature $T_c \ll \Delta E$. Indeed, when restricting to nearest-neighbor hops only, we found glassy behavior even for the simple frustration $f = 3/8$ at large L, unless very slow and careful cooling was used. Such glassy behavior is therefore more a reflection of the frustration being non-trivially dense rather than specifically irrational.

Our results indicate that the "glass transition" observed by Halsey [6] is an artifact of his choice of dynamics. Our observation of an equilibrium first order transition strengthens the analogy to structural glasses and gives a natural explanation for the supercooled relaxation observed by Kim and Lee, whose simulations were carried out for the parameters $f = 13/34$, $L = 34$. Further work is required to investigate whether such a supercooled state can have a well defined finite temperature glass transition below T_c, or whether, as suggested by Granato, this glass transition is at $T = 0$.

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